LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082718\
Data File : VX004264.D
Acq On : 27 Aug 2018 16:17
Operator : JC/MD
Sample : J4662-01
Misc : 5.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-D7-GRAB

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.713	1327	1333	1341	rVB	984405	1630677	1.06%	0.071%
2	9.445	1443	1453	1462	rBV	1543237	2637404	1.71%	0.115%
3	9.561	1466	1472	1478	rBV2	1484540	3023577	1.96%	0.131%
4	9.677	1486	1491	1496	rBV	4329739	7211901	4.68%	0.314%
5	9.890	1519	1526	1534	rVV3	4464840	12457835	8.08%	0.542%
6	9.957	1534	1537	1542	rVB	3648862	5055809	3.28%	0.220%
7	10.067	1548	1555	1560	rBV	7625268	11790516	7.65%	0.513%
8	10.116	1560	1563	1567	rVB2	1332318	1806442	1.17%	0.079%
9	10.177	1567	1573	1579	rBV4	1286589	2640935	1.71%	0.115%
10	10.244	1579	1584	1590	rBV2	3593087	6612675	4.29%	0.288%
11	10.341	1590	1600	1603	rBV2	8465225	18093218	11.74%	0.787%
12	10.384	1603	1607	1610	rVV	9799142	13928719	9.04%	0.606%
13	10.414	1610	1612	1623	rVB2	7777497	14613655	9.48%	0.635%
14	10.518	1623	1629	1635	rBV	6585325	10945213	7.10%	0.476%
15	10.652	1637	1651	1658	rBV2	25611071	65793087	42.69%	2.861%
16	10.737	1658	1665	1669	rBV4	9980976	20953890	13.59%	0.911%
17	10.853	1675	1684	1688	rBV3	39805276	82027875	53.22%	3.567%
18	10.926	1688	1696	1699	rVV2	43593144	83605574	54.24%	3.635%
19	10.963	1699	1702	1707	rVB2	32328539	51379831	33.33%	2.234%
20	11.018	1707	1711	1716	rVB4	12671215	21353132	13.85%	0.928%
21	11.073	1716	1720	1722	rBV2	19593323	28260199	18.33%	1.229%
22	11.103	1722	1725	1729	rVB2	15813985	21308481	13.82%	0.926%
23	11.158	1729	1734	1738	rVB2	29838456	45964746	29.82%	1.999%
24	11.201	1738	1741	1744	rVB	12855888	15114086	9.81%	0.657%
25	11.237	1744	1747	1748	rBV2	6723226	7310758	4.74%	0.318%
26	11.298	1748	1757	1765	rVB4	58768309	127620706	82.80%	5.549%
27	11.371	1766	1769	1771	rBV	7032633	7644611	4.96%	0.332%
28	11.414	1771	1776	1780	rBV3	23193561	44305898	28.74%	1.926%
29	11.463	1780	1784	1787	rBV4	26034964	37377598	24.25%	1.625%
30	11.506	1787	1791	1795	rVV2	37324189	55110390	35.75%	2.396%
31	11.554	1795	1799	1803	rVB3	36567488	58846057	38.18%	2.559%
32	11.597	1803	1806	1811	rVB4	15355753	21379745	13.87%	0.930%
33	11.646	1811	1814	1816	rBV	8031507	10136911	6.58%	0.441%
34	11.707	1816	1824	1828	rVB5	28096169	70373934	45.66%	3.060%

LSC Area Percent Report

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Instrument : MSVOA_X
ClientSampleId : EP1-D7-GRAB

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : SW846 8260

35	11.756	1828	1832	1835	rBV4	19047377	32238986	20.92%	1.402%
36	11.798	1835	1839	1848	rBV6	39847930	95826688	62.17%	4.167%
37	11.920	1854	1859	1862	rBV2	27093848	55037679	35.71%	2.393%
38	11.969	1863	1867	1871	rVB5	36395268	65485785	42.49%	2.847%
39	12.024	1871	1876	1879	rBV2	48198200	77550418	50.31%	3.372%
40	12.115	1886	1891	1894	rBV2	17655470	26231771	17.02%	1.141%
41	12.146	1894	1896	1899	rVB4	13441023	14407604	9.35%	0.626%
42	12.201	1899	1905	1907	rBV5	13275381	27981230	18.15%	1.217%
43	12.237	1909	1911	1915	rVB4	16216579	18652139	12.10%	0.811%
44	12.316	1920	1924	1930	rBV2	35440547	54691569	35.48%	2.378%
45	12.396	1930	1937	1943	rBV4	73687785	154135757	100.00%	6.702%
46	12.475	1946	1950	1951	rBV3	16809170	19673062	12.76%	0.855%
47	12.548	1958	1962	1966	rVB4	30651150	52938059	34.35%	2.302%
48	12.627	1966	1975	1976	rBV5	18340384	34770508	22.56%	1.512%
49	12.688	1981	1985	1992	rVV2	44812872	85140878	55.24%	3.702%
50	12.780	1992	2000	2006	rVV5	23441271	70604109	45.81%	3.070%
51	12.847	2006	2011	2015	rVV5	11331910	24349429	15.80%	1.059%
52	12.896	2015	2019	2024	rVB4	40950509	64808447	42.05%	2.818%
53	12.963	2024	2030	2032	rBV3	28073921	44933938	29.15%	1.954%
54	12.993	2032	2035	2039	rVV2	31277693	40375561	26.19%	1.756%
55	13.030	2039	2041	2043	rVV2	9514844	9989666	6.48%	0.434%
56	13.060	2043	2046	2048	rVV2	22129246	24909962	16.16%	1.083%
57	13.091	2048	2051	2058	rVB2	16702419	28917150	18.76%	1.257%
58	13.158	2058	2062	2067	rBV2	11102779	18686271	12.12%	0.812%
59	13.206	2067	2070	2073	rVB2	9603568	10521547	6.83%	0.457%
60	13.274	2077	2081	2084	rVB2	2993455	4623145	3.00%	0.201%
61	13.316	2084	2088	2091	rBV2	8576613	12552077	8.14%	0.546%
62	13.359	2091	2095	2101	rVB2	38806511	58244952	37.79%	2.532%
63	13.432	2101	2107	2111	rBV2	8976476	13173796	8.55%	0.573%
64	13.481	2111	2115	2119	rVB4	5647949	8805668	5.71%	0.383%
65	13.572	2126	2130	2132	rBV2	3525117	5157043	3.35%	0.224%
66	13.603	2132	2135	2138	rVV2	3874325	5534968	3.59%	0.241%
67	13.645	2138	2142	2146	rVV2	9410080	16113970	10.45%	0.701%
68	13.706	2146	2152	2153	rVV5	3727637	7909173	5.13%	0.344%
69	13.731	2153	2156	2164	rVB2	6438107	10404134	6.75%	0.452%
70	13.810	2164	2169	2173	rBV2	2908560	3931342	2.55%	0.171%
71	13.859	2173	2177	2181	rVB2	2153668	2744911	1.78%	0.119%

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ClientSampleId : EP1-D7-GRAB

Integration Parameters: RTEINT.P
Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Title : SW846 8260

72	13.914	2181	2186	2190	rVB5	1513690	3001055	1.95%	0.130%
73	13.987	2190	2198	2202	rBV4	2110105	4203401	2.73%	0.183%
74	14.273	2240	2245	2253	rVB3	1245164	2349427	1.52%	0.102%

Sum of corrected areas: 2299923360

LSC Report - Integrated Chromatogram

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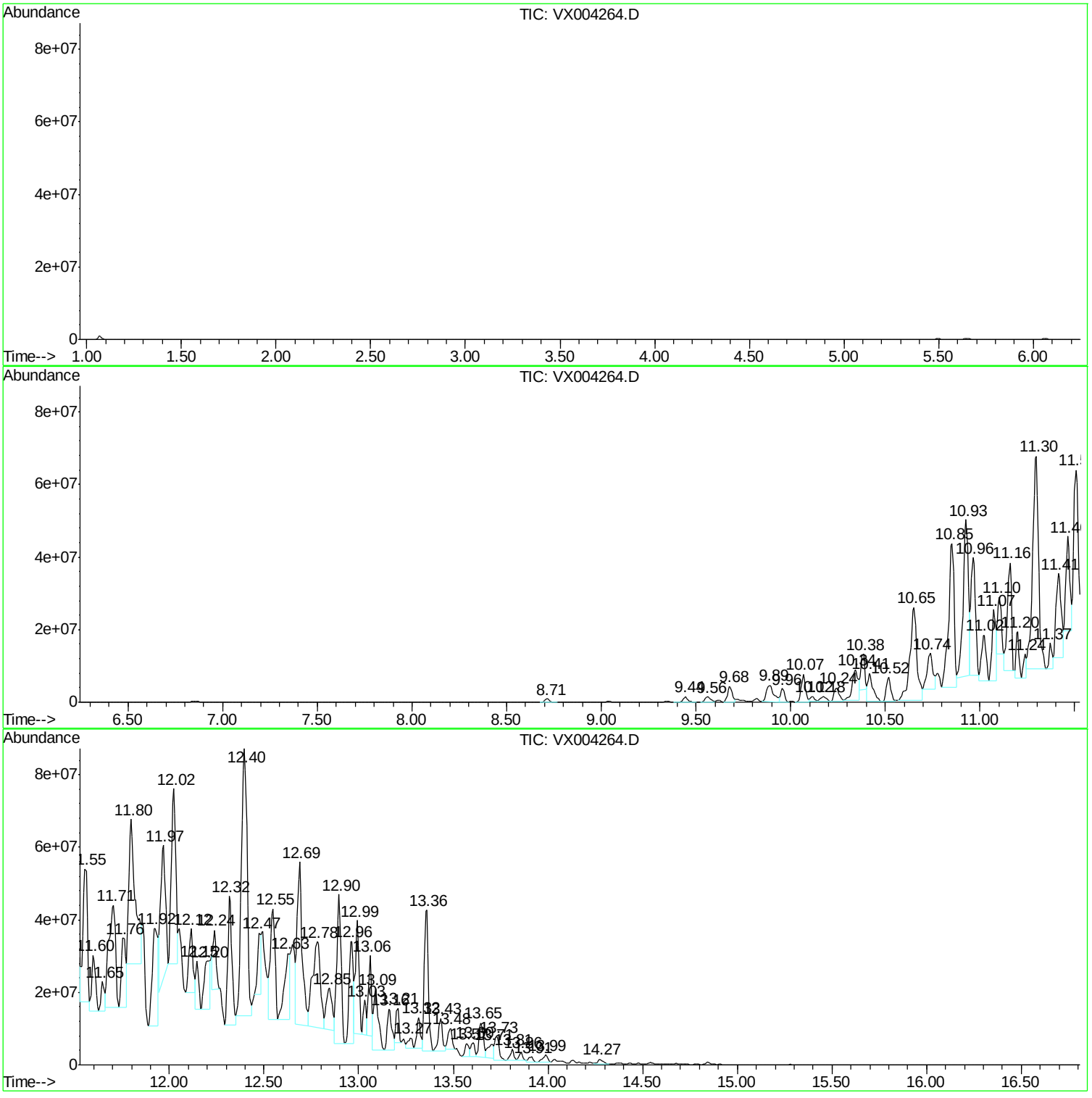
Sample : J4662-01
Misc : 5.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-D7-GRAB

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082718\
Data File : VX004264.D
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Instrument : MSVOA_X
ClientSampleId : EP1-D7-GRAB

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****

Peak Number 1 Cyclohexane, 1,2,4-trimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.89	344.82 ug/l	12457800	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	91
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	81
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	72
4	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	72
5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	70

****

Peak Number 2 Cyclohexane, 1,1,3,5-tetram... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	500.80 ug/l	18093200	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	74
2	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	53
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	52
4	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	46
5	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	43

****

Peak Number 3 cis-1-Ethyl-3-methyl-cycloh... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	385.53 ug/l	13928700	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	90
3	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	90
4	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	78
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	72

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Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Acq On : 27 Aug 2018 16:17
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Sample : J4662-01
Misc : 5.31g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : EP1-D7-GRAB

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	404.49 ug/l	14613700	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	95
2	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
3	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	90
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	87

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Peak Number 5 Cyclopentane, pentyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	302.95 ug/l	10945200	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, pentyl-	140	C10H20	003741-00-2	46
2	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	43
3	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	38
4	3-Hexene, 2-methyl-, (Z)-	98	C7H14	015840-60-5	30
5	3-Hexene, 2-methyl-, (E)-	98	C7H14	000692-24-0	30

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Peak Number 6 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	1821.07 ug/l	65793100	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	62
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	58
3	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	58
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	52
5	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	52

****

Peak Number 7 Nonane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	579.98 ug/l	20953900	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

1	Nonane, 4-methyl-	142	C10H22	017301-94-9 87
2	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3 76
3	Heneicosane	296	C21H44	000629-94-7 50
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3 49
5	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5 47

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Peak Number 8 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	2270.43 ug/l	82027900	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	94
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	90
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
4	Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	64
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59

****

Peak Number 9 Cyclohexane, (1-methylethyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2314.10 ug/l	83605600	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	70
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	62
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	50
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	47
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	47

****

Peak Number 10 Heptane, 3-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	1422.13 ug/l	51379800	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	58
2	Ether, tert-butyl isopropylidene...	154	C10H18O	024524-56-9	47
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45

Library Search Compound Report

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ClientSampleId :
EP1-D7-GRAB

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

4	Heptane, 4-propyl-	142	C10H22	003178-29-8	38
5	2,3-2H-4-Methyl-imidazole-2-one	98	C4H6N2O	039799-77-4	35

Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexane, 1,2,...	9.89	344.8	ug/l	12457800	3	10.12	1806440	50.0
Cyclohexane, 1,1,...	10.34	500.8	ug/l	18093200	3	10.12	1806440	50.0
cis-1-Ethyl-3-met...	10.38	385.5	ug/l	13928700	3	10.12	1806440	50.0
Cyclohexane, 1-et...	10.41	404.5	ug/l	14613700	3	10.12	1806440	50.0
Cyclopentane, pen...	10.52	302.9	ug/l	10945200	3	10.12	1806440	50.0
Cyclohexane, 1-et...	10.65	1821.1	ug/l	65793100	3	10.12	1806440	50.0
Nonane, 4-methyl-	10.74	580.0	ug/l	20953900	3	10.12	1806440	50.0
Octane, 2,6-dimet...	10.85	2270.4	ug/l	82027900	3	10.12	1806440	50.0
Cyclohexane, (1-m...	10.93	2314.1	ug/l	83605600	3	10.12	1806440	50.0
Heptane, 3-ethyl-...	10.96	1422.1	ug/l	51379800	3	10.12	1806440	50.0